

# Synchrotrons for condensed matter physics and materials science: Research snippets and an outlook

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# Magnetic & electronic phase transitions at high pressure

# Antiferromagnetism in chromium

VOLUME 19, NUMBER 15

PHYSICAL REVIEW LETTERS

9 OCTOBER 1967

## PRESSURE DEPENDENCE OF ITINERANT ANTIFERROMAGNETISM IN CHROMIUM

D. B. McWhan and T. M. Rice

Bell Telephone Laboratories, Murray Hill, New Jersey

(Received 9 August 1967)

The Néel temperature of Cr is found to vary exponentially with volume support of a two-band model of itinerant antiferromagnetism. The tendency of the magnetic contribution to the electrical resistivity can be taken into account only the variation in the number of effective carriers in the presence of a band gap ( $2\Delta$ ) due to the magnetic ordering. The ratio  $\Delta_0/kT_N$  is 2.3 at  $P = 26$  kbar.

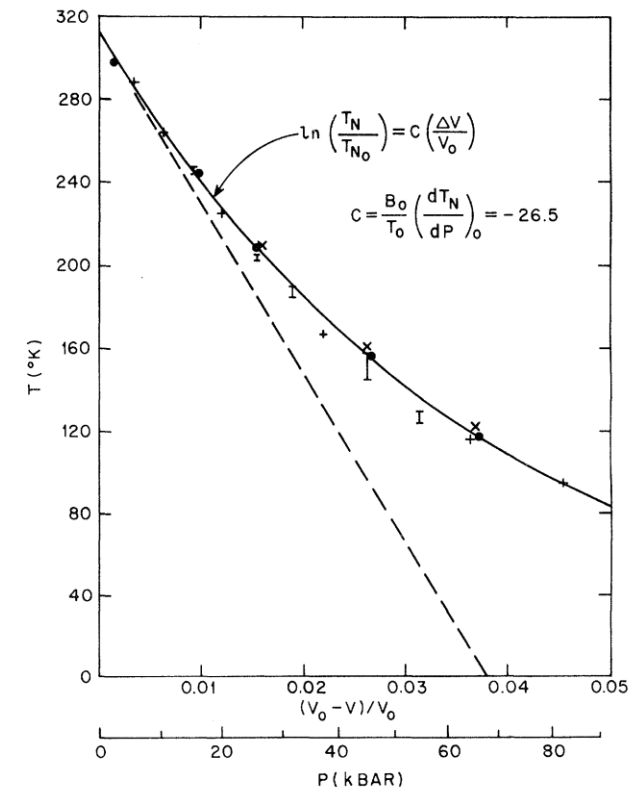


FIG. 1. Volume dependence of the Néel temperature of chromium. Vertical bars, sample 1; crosses, sample 2; and solid circles, sample 3.

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PHYSICAL REVIEW B

VOLUME 51, NUMBER 16

## X-ray-scattering study of charge- and spin-density waves in chromium

J. P. Hill, G. Helgesen,\* and Doon Gibbs

Department of Physics, Brookhaven National Laboratory, Upton, New York 11973

(Received 28 September 1994; revised manuscript received 19 December 1994)

We report an x-ray-scattering study of the incommensurate modulations in pure chromium. X-ray magnetic scattering from the spin-density wave (SDW) is observed. No resonant enhancement of the signal is obtained near the Cr  $K$  edge. On cooling through the spin-flip transition, the magnetic signal goes to zero, consistent with the polarization dependence of nonresonant magnetic scattering and the known polarization of the SDW. Charge scattering is observed at the second harmonic due to the associated charge-density wave (CDW). The intensity of the second harmonic is unchanged on cooling through the spin-flip transition. A survey of possible second-harmonic satellites reveals that a single  $Q$  state exists in the near-surface region. The amplitude of the lattice distortion is estimated to be  $(\Delta_2/a) = 1.5 \pm 0.2 \times 10^{-3}$ , consistent with published reports. A fourth harmonic is also observed, suggesting that the CDW is not perfectly sinusoidal. The intensity of the fourth harmonic is 0.05% of the second and we find  $(\Delta_4/a) = 2.8 \pm 0.2 \times 10^{-5}$ . The temperature dependence of the charge harmonics is found to obey mean-field scaling.

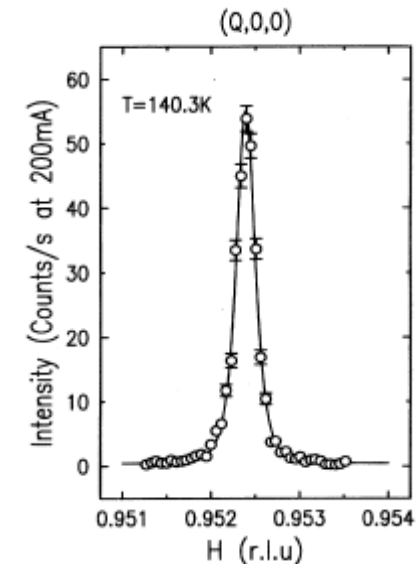
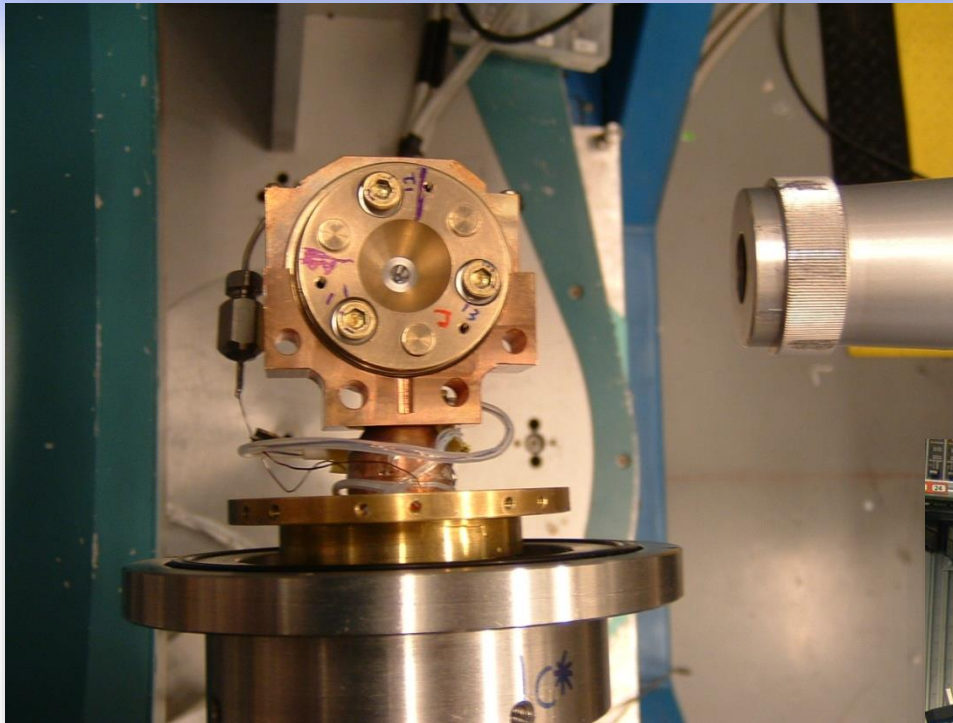


FIG. 2. Longitudinal scan through the SDW peak. These data were taken on a wiggler beamline at  $E = 5.91$  keV, just below the Cr  $K$  edge at  $T = 140.3$  K.

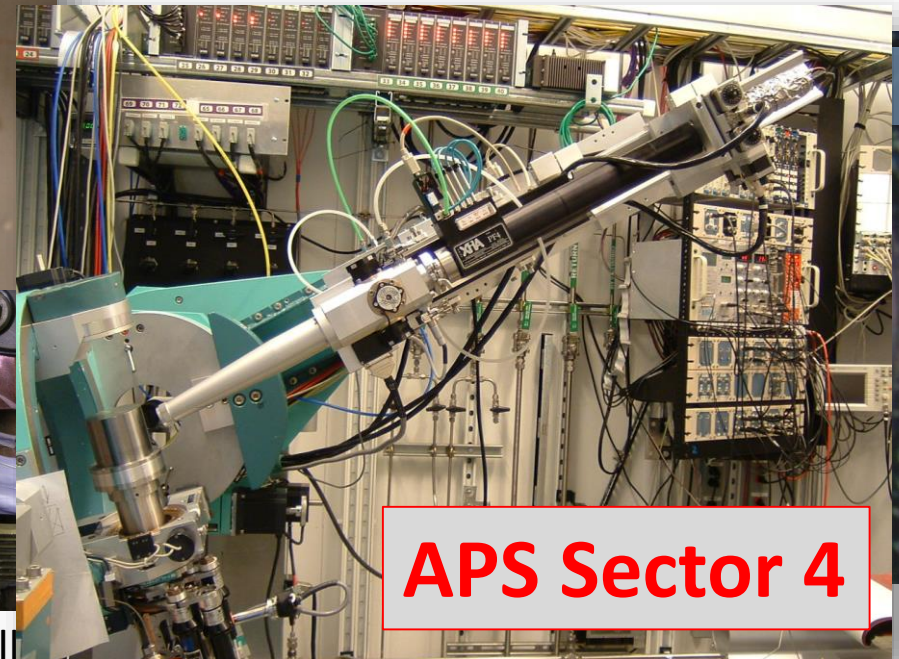
# Experiment – High Pressure X-Ray Diffraction



order parameters  
quantum phase transition  
diamond anvil cell



Diffraction geometry;  
sample in purple



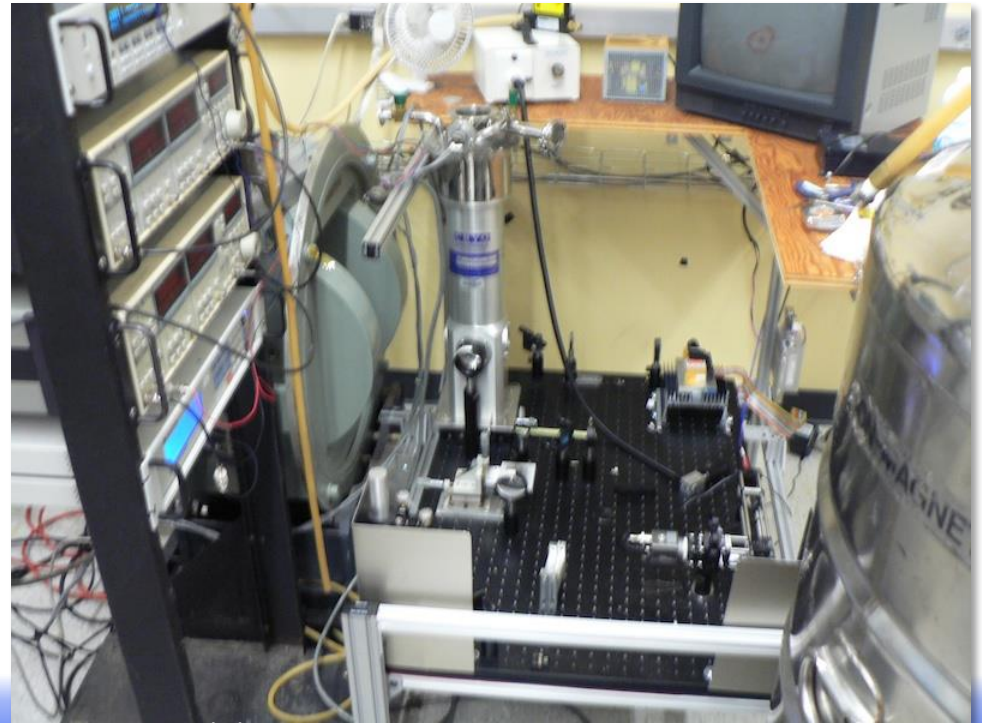
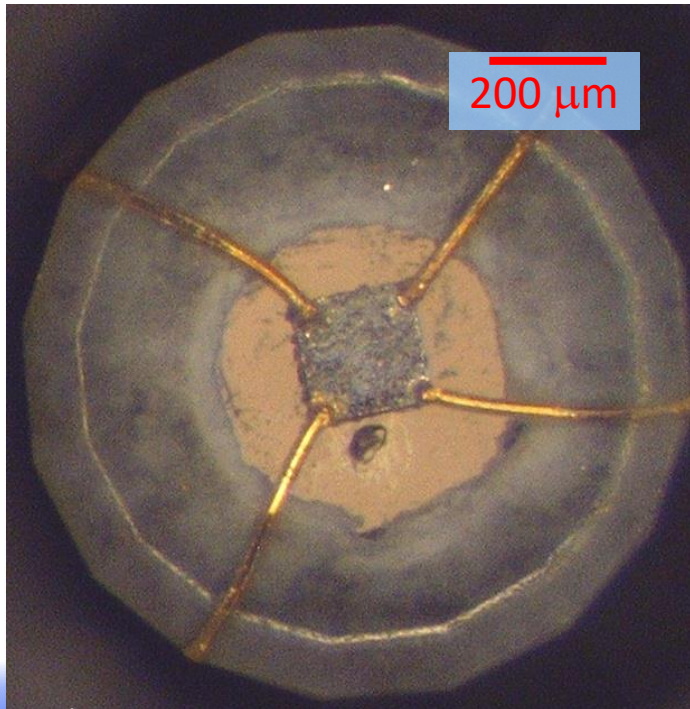
Pressure cell  
cryostat cold finger

chamber



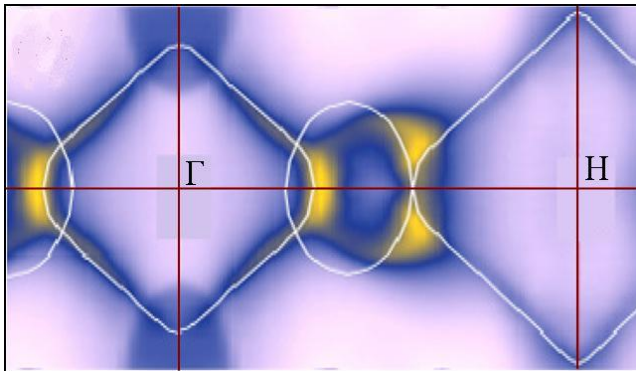
# Experiment – High Pressure Transport

- Resistivity + Hall coefficient
  - Sensitive to metallic DOS
  - Carrier scattering from critical fluctuations
- Magnetotransport in a DAC
  - van der Pauw geometry  $\rightarrow$  four leads in the sample chamber
  - Magnetic field + fluorescence spectrometry + *in situ* pressure control



# Ground state of antiferromagnetic chromium

- Equation for exchange field is analogous to the BCS gap equation
- SDW remains stable for arbitrarily weak interaction provided that the nested phase space remains large



Photoemission measurement of paramagnetic Fermi surface in (011) plane; Rotenberg *et al.*, New J. Phys. **7**, 114 (2005).

exchange field

interaction

$\theta$  = mixing angle  
(depends on  $g$ )

$$g_0(k') = \int \frac{d^3k}{8\pi^3} \frac{4\pi e^2}{|k - k'|^2} \cos \theta \sin \theta$$

- replace interaction with a constant
- model two nested bands
- expand for small  $g/E_F$

$$g_0 \propto T_N \propto e^{-1/\lambda}, \quad \lambda = \frac{\gamma^2 V k_c^2}{2\pi^2 v}$$

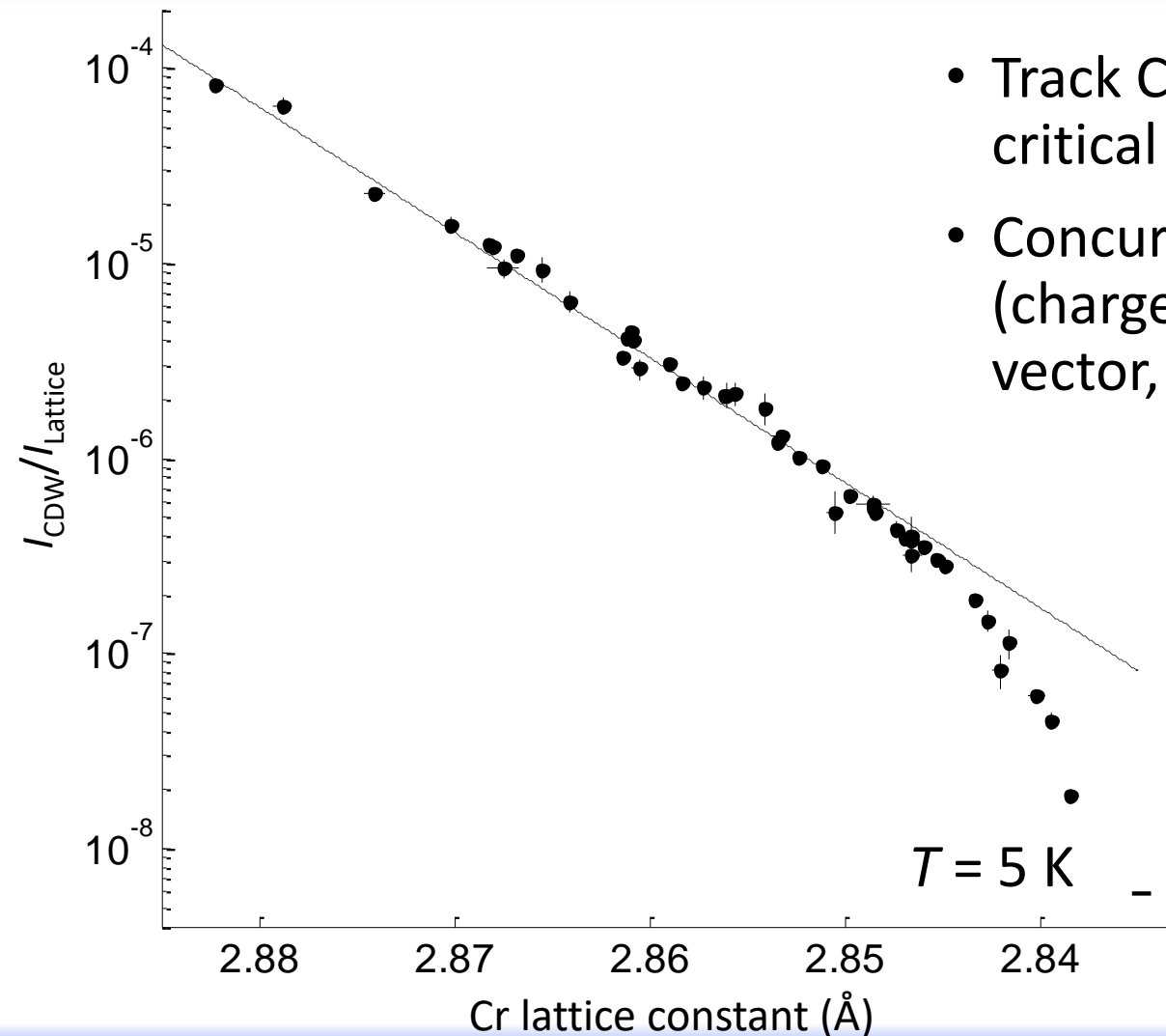
$\gamma$  = exchange integral

$V$  = Coulomb potential

$4\pi k_c^2$  = nesting area

$v$  = average Fermi velocity

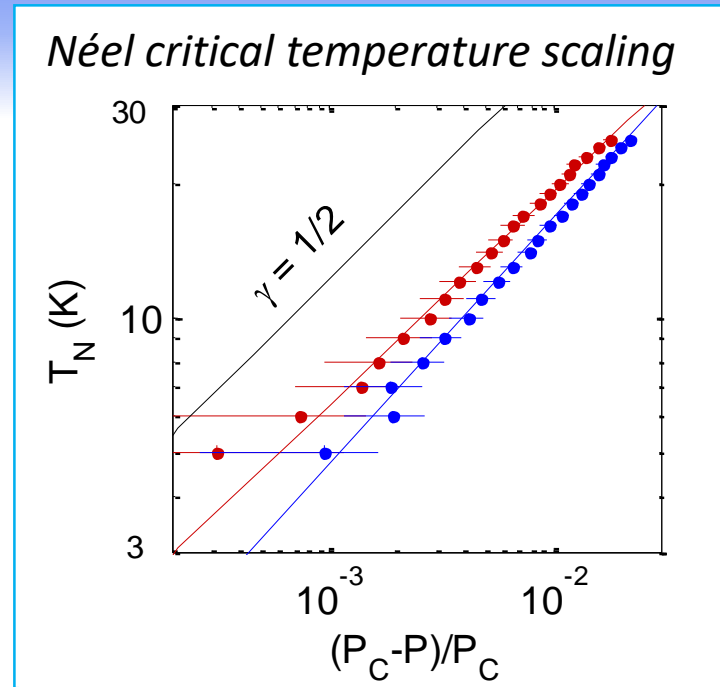
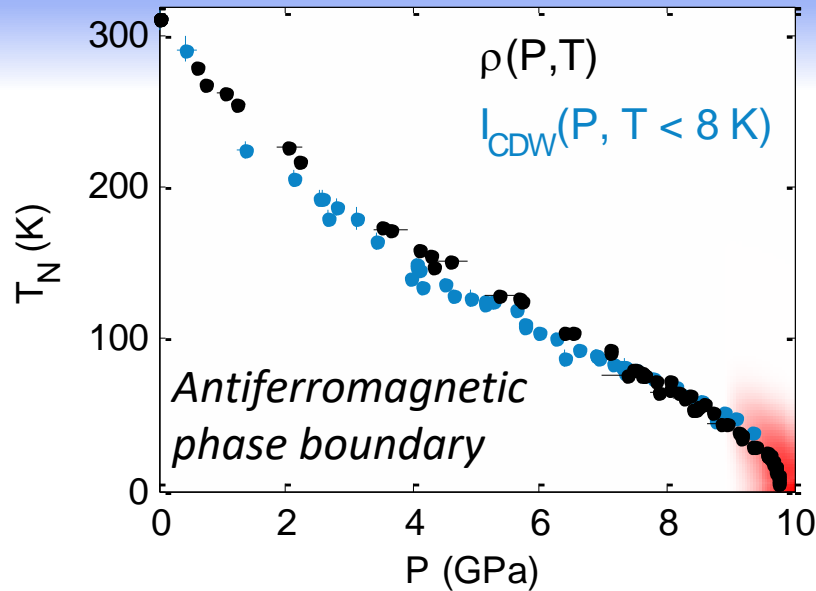
# Weak-coupling ground state and the quantum critical regime



- Track CDW diffraction into the critical regime
- Concurrent measurement of (charge) order parameter,  $Q$ -vector, and crystal structure



# Combined X-ray and electrical results



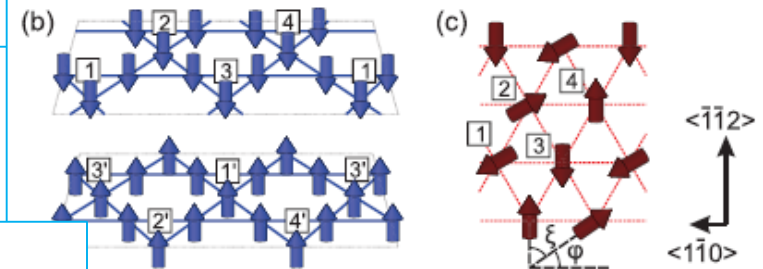
- Electrical results support phase diagram determined by CDW diffraction
- Measure scaling relationships between pressure,  $T_N$ , resistivity, and Hall coefficient
  - *All consistent with mean-field Fermi surface reconstruction*

# Technique development is enabling!

PHYSICAL REVIEW B 86, 014422 (2012)

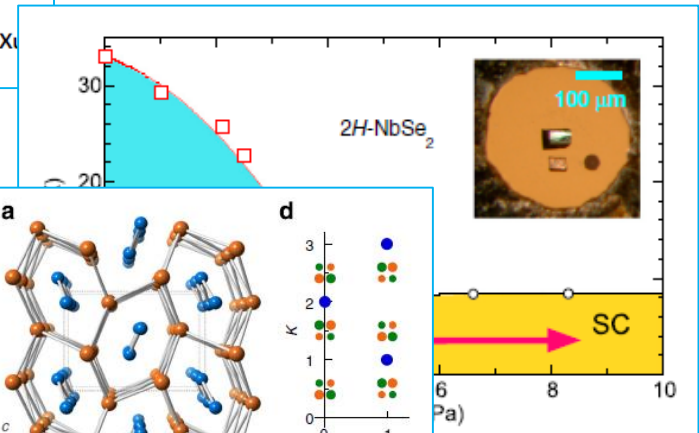
## Pressure tuning of competing magnetic interactions in intermetallic CeFe<sub>2</sub>

Jiyang Wang,<sup>1</sup> Yejun Feng,<sup>1,2,\*</sup> R. Jaramillo,<sup>3</sup> Jasper van Wezel,<sup>4</sup>  
P. C. Canfield,<sup>5</sup> and T. F. Rosenbaum<sup>1</sup>



## Order parameter fluctuations at a buried quantum critical point

Yejun Feng<sup>a,b,1</sup>, Jiyang Wang<sup>b</sup>, R. Jaramillo<sup>c</sup>, Jasper van Wezel<sup>d</sup>, S. Haravifard<sup>a,b</sup>, G. Srajer<sup>a</sup>, Y. Liu<sup>e,f</sup>, Z.-A. Xu<sup>g</sup>, P. B. Littlewood<sup>g</sup>, and T. F. Rosenbaum<sup>b,1</sup>



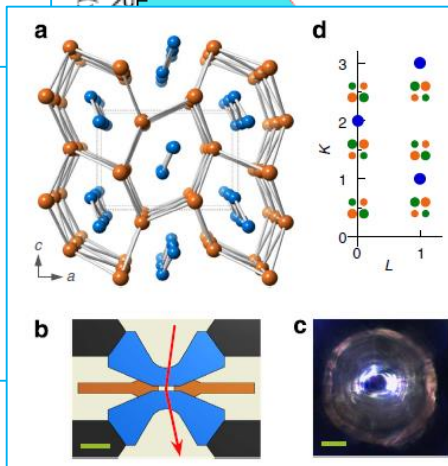
## ARTICLE

Received 29 Mar 2014 | Accepted 27 May 2014 | Published 18 Jun 2014

DOI: 10.1038/ncomms5218

## Hidden one-dimensional spin modulation in a three-dimensional metal

Yejun Feng<sup>1,2</sup>, Jiyang Wang<sup>2</sup>, A. Palmer<sup>2</sup>, J.A. Aguiar<sup>3</sup>, B. Mihaila<sup>3,4</sup>, J.-Q. Yan<sup>5,6</sup>, P.B. Littlewood<sup>2,7</sup>  
& T.F. Rosenbaum<sup>2</sup>







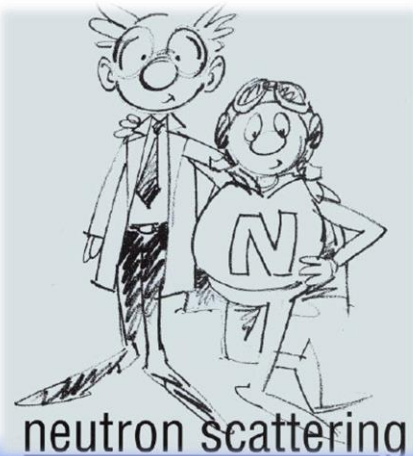
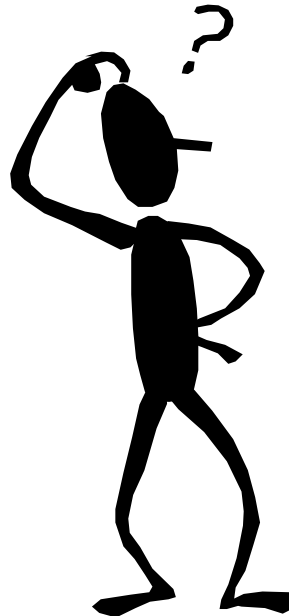
Tom Rosenbaum (Caltech)  
Yejun Feng (Okinawa Institute of Sci. and Tech.)  
Jonathan Lang (Argonne)  
George Srajer (Argonne)

PNAS **107**, 13631 (2010)  
J. Appl. Phys. **107**, 09E116 (2010)  
Rev. Sci. Instrum **81**, 041301 (2010)  
Nature **459**, 405 (2009)  
Phys. Rev. B **77**, 184418 (2008)  
Phys. Rev. Lett. **99**, 137201 (2007)

# Opportunities for synchrotrons in materials science



# A user's perspective



neutron scattering





# Unassailable advantages of X-rays

## 1. Contrast modes

Collective  
excitations

Fast dynamics

Slow dynamics

Crystallography

Morphology

Composition

Chemistry

Local structure

Bandstructure &  
quasiparticle  
spectroscopy

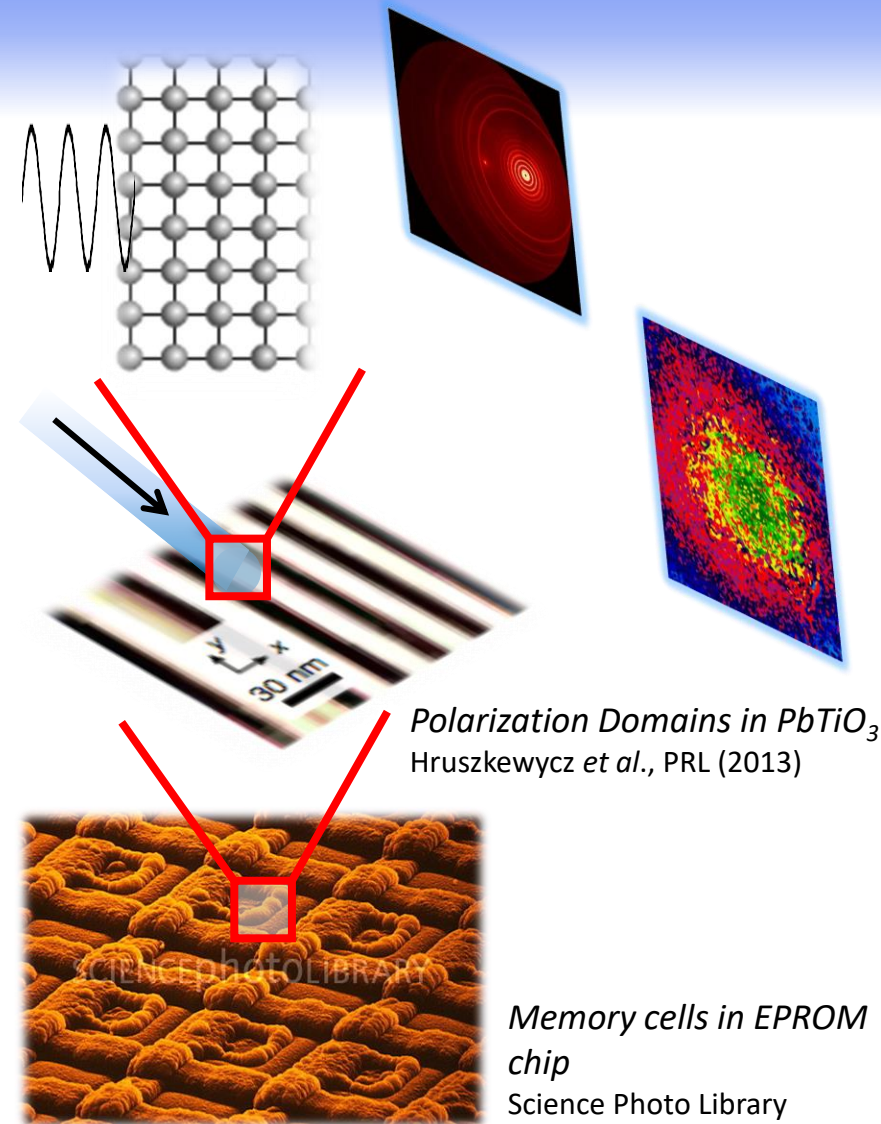
# Unassailable advantages of X-rays

## 2. Field of view

Atomic scale  $\leftrightarrow$  X-ray wavelength

Macroscale  $\leftrightarrow$  Scanning probe

Mesoscale  $\leftrightarrow$  Focused beam



# Unassailable advantages of (hard) X-rays

## 3. *In situ* capabilities

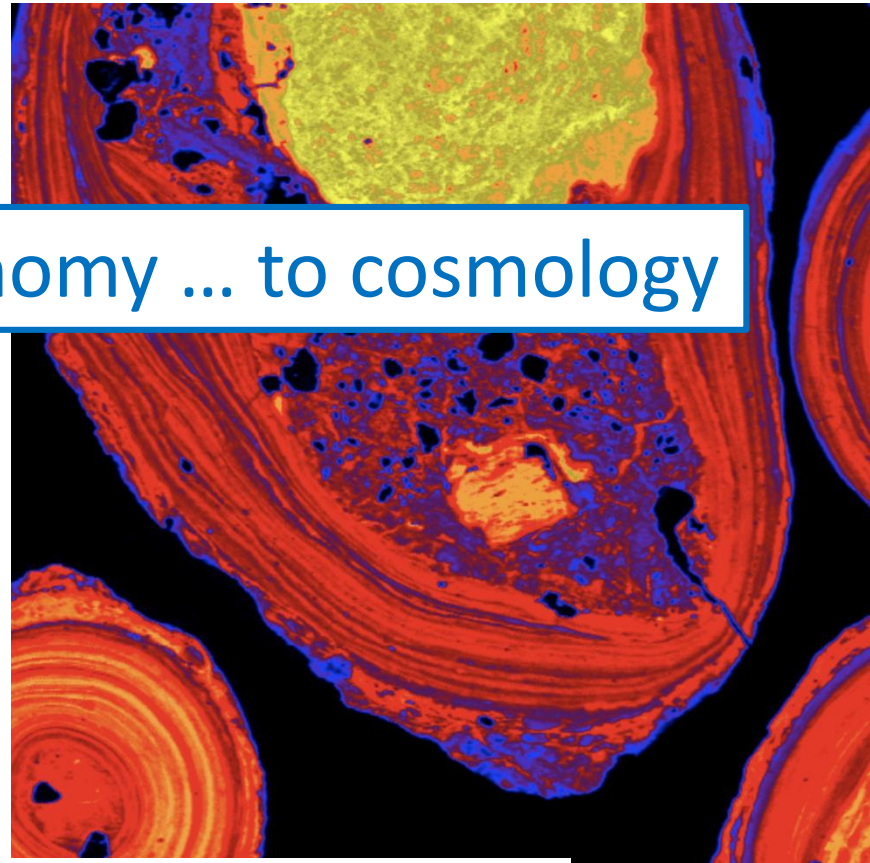
	PVD/CVD	Micro-electronics	Solar Cell	Thermo-electrics	Catalysis	Batteries	Fuel Cell
Temperature (°C)	300-600	0-300	500-1500	500-1000	400-2000	~500	600-1000
Pressure	$10^{-8}$ – 1 atm	1 atm	1 atm	1 atm	1 atm	1 atm	1-5 atm
Length Scale (Defect - Device)	Å - μm	nm - cm	nm - cm	nm - cm	Å - cm	nm - mm	nm - mm

# The importance of field-of-view

Standard (1500ms/pt)  
step scan, 10  $\mu\text{m}/\text{pixel}$   
0.8 x 0.8 mm<sup>2</sup>



Multichannel detector (5ms/pt)  
slew scan, 10  $\mu\text{m}/\text{pixel}$   
13.5 x 13.5 mm<sup>2</sup>



From astronomy ... to cosmology

Data from studies and related  
presentations of:

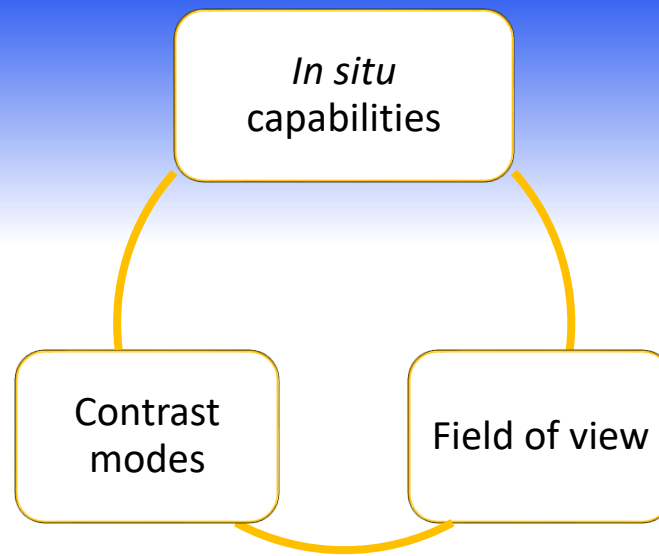
D.P. Siddons *et al.*

DOI: 10.1017/S1431927605510298

C.G. Ryan *et al.*

DOI: 10.1016/j.nima.2009.11.035

Iron-oxide nodules, Rose Dam, WA

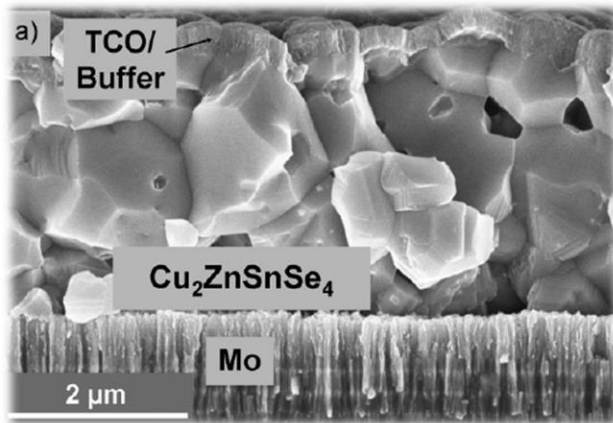


# Combining these advantages...



# Spectromicroscopy & mesoscale electronic heterogeneity

- Correlate composition, spectra & function in inhomogeneous materials
- Compound semiconductors
  - Thin film photovoltaics

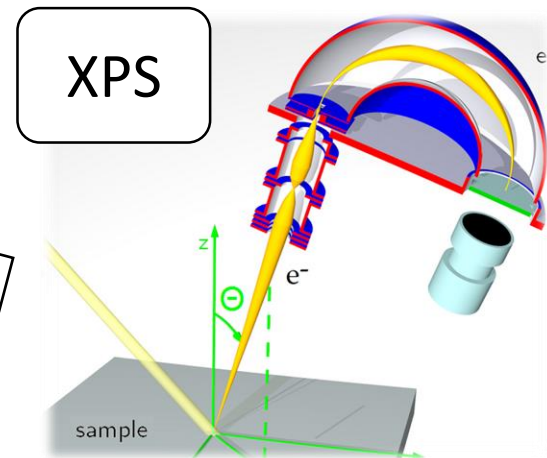


CZTS solar cell

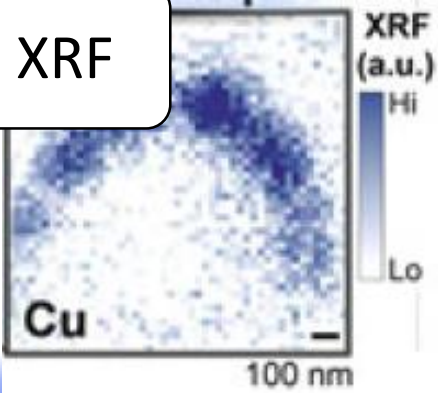
Todorov *et al.*, Adv. Mater. **22**, E156 (2010).

Electronic structure

Composition fluctuations



XPS



XRF

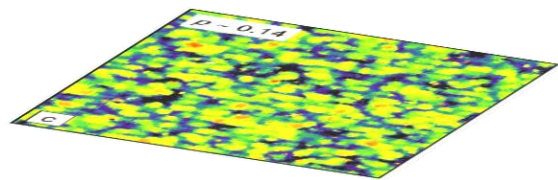
*In situ*  
capabilities

Contrast  
modes

Field of  
view

# Spectromicroscopy & mesoscale electronic heterogeneity

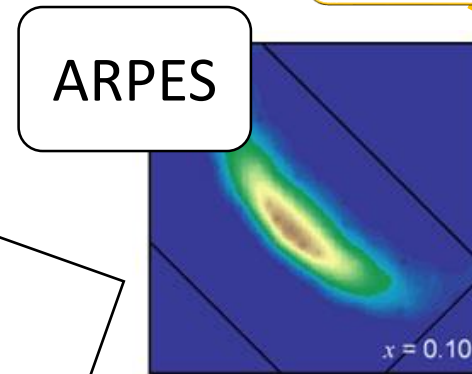
- Correlate composition, spectra & function in inhomogeneous materials
- Correlated oxides
  - High- $T_c$  cuprates
  - Manganites



Inhomogeneous pseudogap in BSCCO  
Slezak *et al.*, MRS Bull. **30**, 437 (2005)

Quasiparticle spectroscopy

Magnon spectroscopy



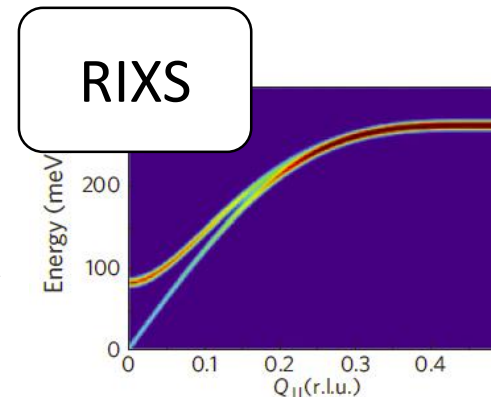
ARPES

Contrast modes

Field of view

*In situ* capabilities

Zhi-Xun Chen

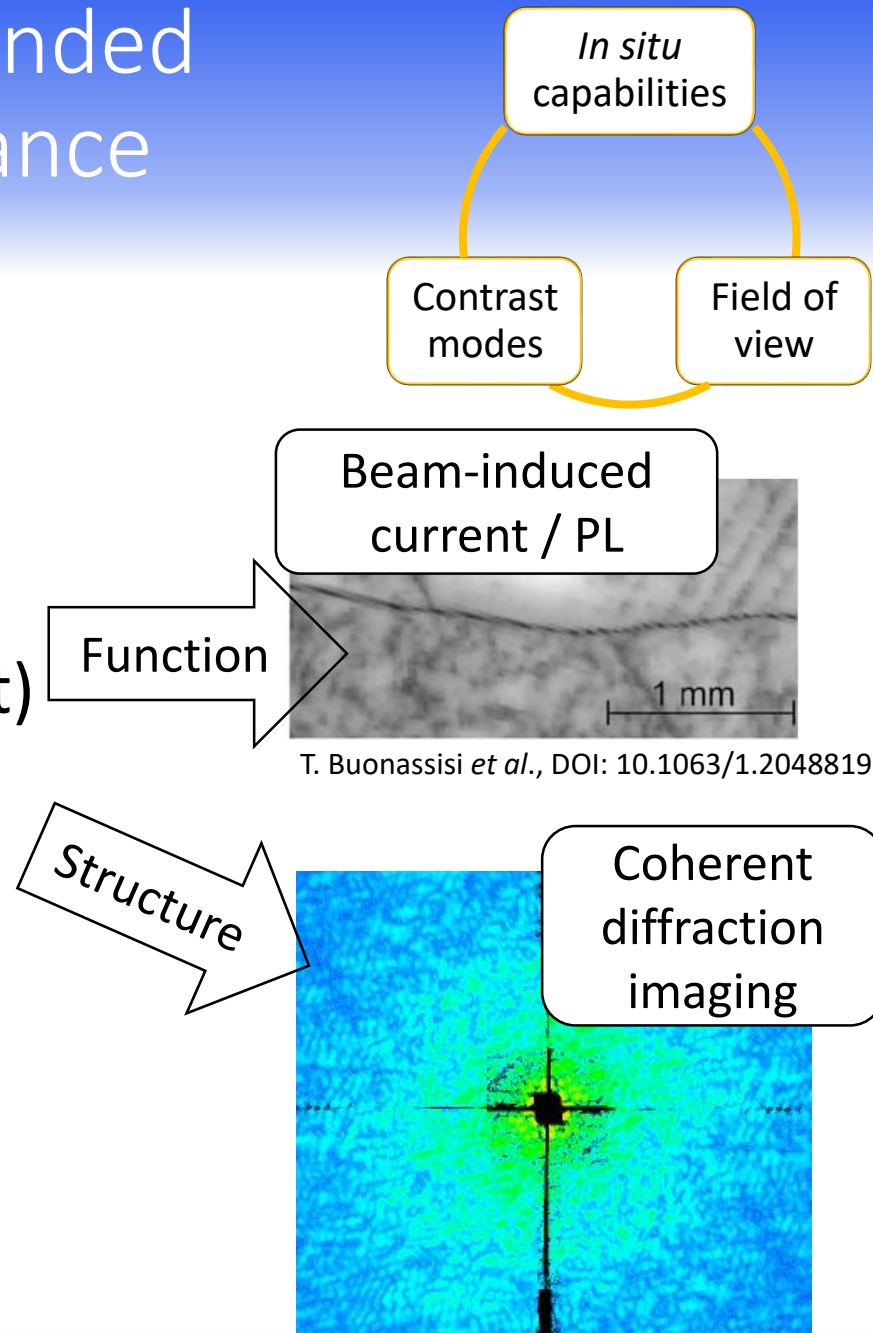


RIXS

Le Tacon *et al.*, Nat. Phys. **7**, 725 (2011)

# Materials processing, extended defects & device performance

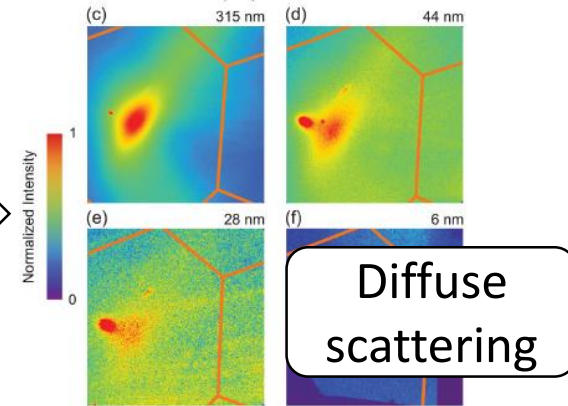
- Microscopic view of materials synthesis & processing
- Connect structure of extended defects to function (PL, current)
- Applications in
  - Heteroepitaxy (*e.g.* III-V on Si)
  - Passivation
  - Degradation & failure analysis



# Heat transport and non-equilibrium device physics

- Microscopic understanding of heat generation & transport
  - Phonon spectra in confined & disordered materials
  - Interface resistance
  - Ballistic & diffusive transport
- Outstanding questions in
  - Thermoelectrics
  - Thermal management
  - Microelectronics scaling

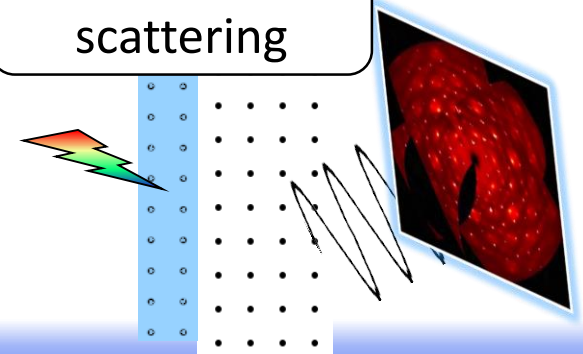
Nanoprobe  
thermometry



Gopalakrishnan *et al.*, Phys. Rev. Lett.  
**110**, 205503 (2013)

Thermal  
interfaces

Pump-probe  
scattering



*Warning: Incoherent  
flux ahead*

# Thoughts on building productive institutional relationships



# From CATs and super-users ... to “just” another tool in the materials science kit

## The olden days

- Beamlines built and run by collaborative access teams (CATs), with significant university involvement
- PIs were often synchrotron super-users and formed strong relationships with CATs

## Today

- Expense and scope of beamline development prices out the CAT model and creates incentive to broaden user base
- User facility model now includes expectation of ease-of-use and quick answers

# Synchrotron ambassadors

- Who are the synchrotron ambassadors at MIT?
  - In this room
  - Busy
- Who are the X-ray ambassadors at MIT?
  - XRD facility managers



X-ray Diffraction Shared Experimental Facility

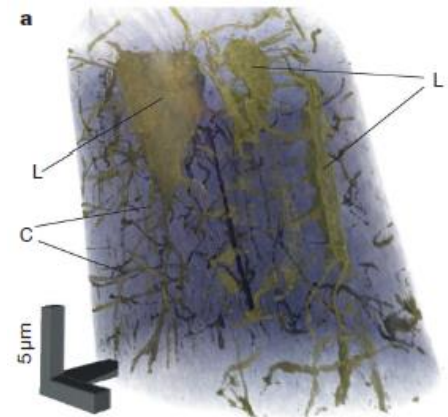
- What is the role of a synchrotron ambassador?

Turning hero experiments ... → ... into metrology

  - Electron microscopy community seems better at this

# Success hinges on usability

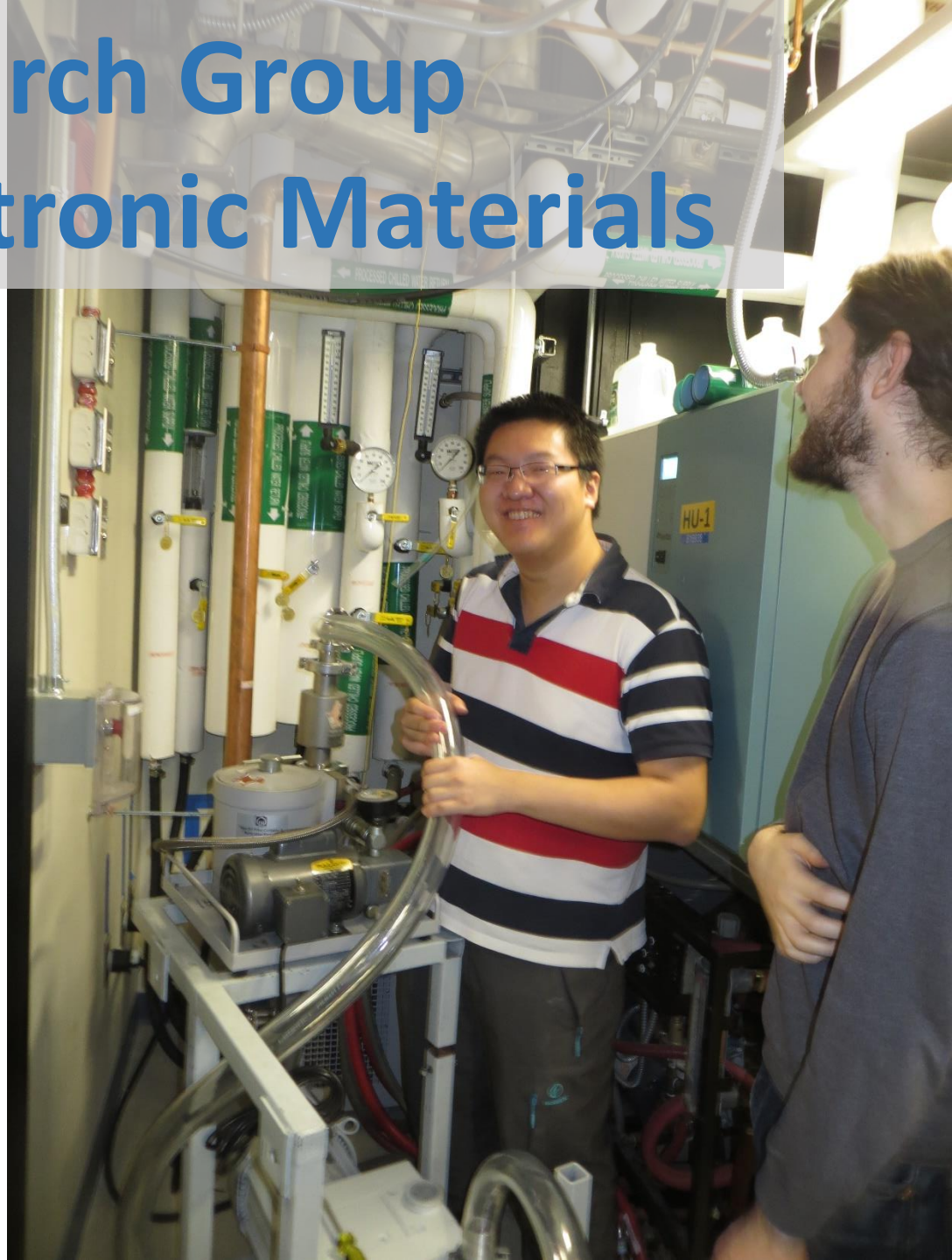
- Success will hinge on all aspects of the tool
  - Spot size and coherence are enabling factors
  - End-station usability
  - Superb sample environments
  - Accessible, specialized and powerful computing
- Lens-less imaging (ptychography + tomography) must become standard
  - Near-term: everyone should be able to do it, given an honest effort (like Reitvelt refinement?)
  - Medium-term: everyone should be able to do it, given minimal effort (like SEM?)



Dierolf *et al.*, Nature **467**, 436 (2010)

# Jaramillo Research Group

## Electronic Materials



# Opportunities in chalcogenide electronic materials

## **Sensing**

- Defect-engineering to customize photoresponse
- Alternative processes for sulfide & selenide film growth for IR

## **Neuromorphic**

- Excitation & inhibition of opto-electronic contrast through defect-engineering

## **Photovoltaics & photochemistry**

- Defect-tolerant semiconductor alloys with tunable band gap

## **Solid state chemistry & physics**

- Chalcogenide perovskites & similarly complex, ionic structures

